

chain nodes :

1 2 4 5 7 8 22 23 24 25 26 40 41 43 44 45 46 47 48

ring nodes :

10 11 12 13 14 15 16 17 18 19 20 21 28 29 30 31 32 33 34 35 36 37  
38 39

chain bonds :

1-2 1-5 2-4 5-8 5-7 10-22 11-23 19-22 23-24 23-25 23-26 32-40 37-40 38-43  
43-44 44-45 45-46 45-47 47-48

ring bonds :

10-11 10-15 11-12 12-13 13-14 14-15 16-17 16-21 17-18 18-19 19-20 20-21 28-29  
28-33 29-30 30-31 31-32 32-33 34-35 34-39 35-36 36-37 37-38 38-39

exact/norm bonds :

1-2 1-5 2-4 5-8 5-7 10-22 11-23 19-22 23-24 23-25 23-26 32-40 37-40 43-44  
44-45 45-46 45-47 47-48

exact bonds :

38-43

normalized bonds :

10-11 10-15 11-12 12-13 13-14 14-15 16-17 16-21 17-18 18-19 19-20 20-21 28-29  
28-33 29-30 30-31 31-32 32-33 34-35 34-39 35-36 36-37 37-38 38-39

isolated ring systems :

containing 10 : 16 : 28 : 34 :

1:0,S

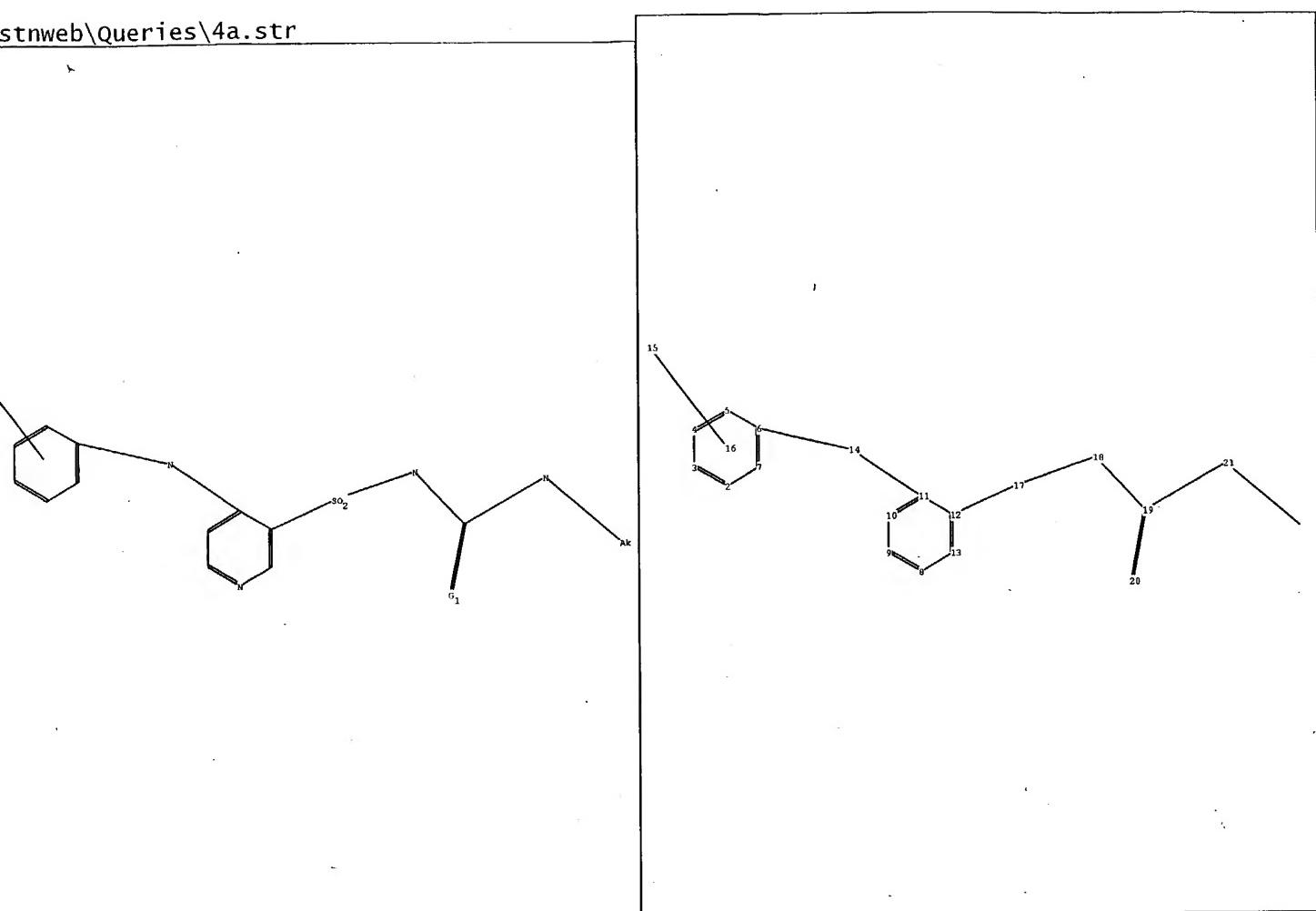
2:CH3,ET

atcat level :

1:CLASS 2:CLASS 4:CLASS 5:CLASS 7:CLASS 8:CLASS 10:Atom 11:Atom 12:Atom 13:Atom  
14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:CLASS  
23:CLASS 24:CLASS 25:CLASS 26:CLASS 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom  
33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:CLASS 41:CLASS  
42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS

fragments assigned reactant role:

containing 1  
containing 10  
ragments assigned product role:  
containing 28



ain nodes :  
14 15 17 18 19 20 21 22

ng nodes :  
2 3 4 5 6 7 8 9 10 11 12 13

ain bonds :  
6-14 11-14 12-17 17-18 18-19 19-20 19-21 21-22

ng bonds :  
2-3 2-7 3-4 4-5 5-6 6-7 8-9 8-13 9-10 10-11 11-12 12-13

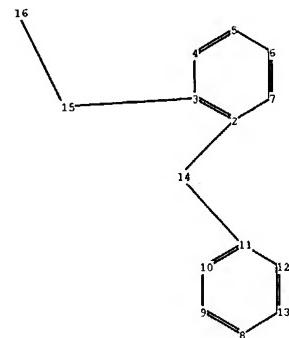
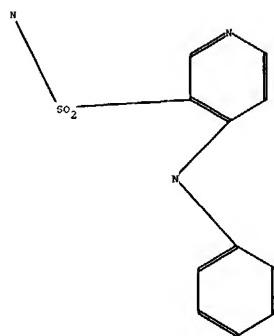
act/norm bonds :  
6-14 11-14 17-18 18-19 19-20 19-21 21-22

act bonds :  
12-17

ormalized bonds :  
2-3 2-7 3-4 4-5 5-6 6-7 8-9 8-13 9-10 10-11 11-12 12-13

0,S

ch level :  
2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom  
13:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS  
22:CLASS



chain nodes :

14 15 16

ring nodes :

2 3 4 5 6 7 8 9 10 11 12 13

chain bonds :

2-14 3-15 11-14 15-16

ring bonds :

2-3 2-7 3-4 4-5 5-6 6-7 8-9 8-13 9-10 10-11 11-12 12-13

exact/norm bonds :

2-14 11-14 15-16

exact bonds :

3-15

normalized bonds :

2-3 2-7 3-4 4-5 5-6 6-7 8-9 8-13 9-10 10-11 11-12 12-13

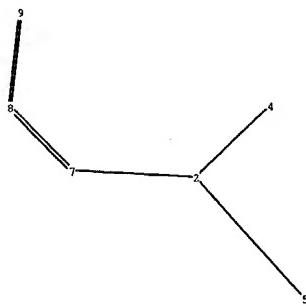
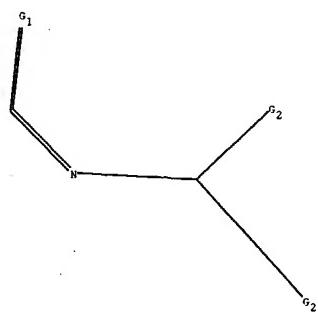
isolated ring systems :

containing 2 : 8 :

51:0,S

Match level :

2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom  
13:Atom 14:CLASS 15:CLASS 16:CLASS



chain nodes :

2 4 5 7 8 9

chain bonds :

2-4 2-5 2-7 7-8 8-9

exact/norm bonds :

2-4 2-5 2-7 7-8 8-9

G1:0,S

G2:CH3,Et

Match level :

2:CLASS 4:CLASS 5:CLASS 7:CLASS 8:CLASS 9:CLASS

\* \* \* \* \* \* \* \* \* \* Welcome to STN International \* \* \* \* \* \* \* \* \* \*

<u>NEWS</u>	<u>1</u>	Web Page URLs for STN Seminar Schedule - N. America
<u>NEWS</u>	<u>2</u>	"Ask CAS" for self-help around the clock
<u>NEWS</u>	<u>3</u>	EXTEND option available in structure searching
<u>NEWS</u>	<u>4</u>	Polymer links for the POLYLINK command completed in REGISTRY
<u>NEWS</u>	<u>5</u>	New UPM (Update Code Maximum) field for more efficient patent SDIs in CAplus
<u>NEWS</u>	<u>6</u>	CAplus super roles and document types searchable in REGISTRY
<u>NEWS</u>	<u>7</u>	Additional enzyme-catalyzed reactions added to CASREACT
<u>NEWS</u>	<u>8</u>	ANTE, AQUALINE, BIOENG, CIVILENG, ENVIROENG, MECHEENG, and WATER from CSA now available on STN(R)
<u>NEWS</u>	<u>9</u>	BEILSTEIN enhanced with new display and select options, resulting in a closer connection to BABS
<u>NEWS</u>	<u>10</u>	BEILSTEIN on STN workshop to be held August 24 in conjunction with the 228th ACS National Meeting
<u>NEWS</u>	<u>11</u>	IFIPAT/IFIUDB/IFICDB reloaded with new search and display fields
<u>NEWS</u>	<u>12</u>	CAplus and CA patent records enhanced with European and Japan Patent Office Classifications
<u>NEWS</u>	<u>13</u>	STN User Update to be held August 22 in conjunction with the 228th ACS National Meeting
<u>NEWS</u>	<u>14</u>	The Analysis Edition of STN Express with Discover! (Version 7.01 for Windows) now available
<u>NEWS</u>	<u>15</u>	Pricing for the Save Answers for SciFinder Wizard within STN Express with Discover! will change September 1, 2004
<u>NEWS</u>	<u>16</u>	BIOCOMMERCE: Changes and enhancements to content coverage
<u>NEWS</u>	<u>17</u>	BIOTECHABS/BIOTECHDS: Two new display fields added for legal status data from INPADOC
<u>NEWS</u>	<u>18</u>	INPADOC: New family current-awareness alert (SDI) available
<u>NEWS</u>	<u>19</u>	New pricing for the Save Answers for SciFinder Wizard within STN Express with Discover!

NEWS EXPRESS JULY 30 CURRENT WINDOWS VERSION IS V7.01, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004

**NEWS HOURS**      STN Operating Hours Plus Help Desk Availability

## NEWS INTER General Internet Information

NEWS LOGIN      Welcome Banner and News Items

NEWS PHONE: Direct Dial and Telecommunication Network Access to SIR

NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 16:15:40 ON 01 SEP 2004

=> file reg  
COST IN U.S. DOLLARS  
  
FULL ESTIMATED COST

SINCE FILE ENTRY	TOTAL SESSION
0.21	0.21

FILE 'REGISTRY' ENTERED AT 16:15:45 ON 01 SEP 2004  
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STRUCTURE FILE UPDATES: 31 AUG 2004 HIGHEST RN 736193-62-7  
 DICTIONARY FILE UPDATES: 31 AUG 2004 HIGHEST RN 736193-62-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when  
 conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
 information enter HELP PROP at an arrow prompt in the file or refer  
 to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> file casreact	SINCE FILE	TOTAL
COST IN U.S. DOLLARS	ENTRY	SESSION
FULL ESTIMATED COST	3.78	3.99

FILE 'CASREACT' ENTERED AT 16:21:07 ON 01 SEP 2004  
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 26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 29 Aug 2004 VOL 141 ISS 9

```
*****
*          *
*      CASREACT now has more than 8 million reactions      *
*          *
*****
```

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991)  
 provided by InfoChem, INPI data prior to 1986, and Biotransformations  
 database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance  
 identification.

```
=>
L1      STRUCTURE UPLOADED

=> d 11
L1 HAS NO ANSWERS
L1      STR

=> s 11
```

SAMPLE SEARCH INITIATED 16:21:47 FILE 'CASREACT'  
 SCREENING COMPLETE - 4 REACTIONS TO VERIFY FROM 1 DOCUMENTS

100.0% DONE 4 VERIFIED 1 HIT RXNS 1 DOCS  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*

PROJECTED VERIFICATIONS: 4 TO 199  
 PROJECTED ANSWERS: 1 TO 79

L2 1 SEA SSS SAM L1 ( 1 REACTIONS)

=> s 11 full  
 THE ESTIMATED SEARCH COST FOR FILE 'CASREACT' IS 102.30 U.S. DOLLARS  
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y  
 FULL SEARCH INITIATED 16:21:51 FILE 'CASREACT'  
 SCREENING COMPLETE - 11 REACTIONS TO VERIFY FROM 5 DOCUMENTS

100.0% DONE 11 VERIFIED 4 HIT RXNS 4 DOCS  
 SEARCH TIME: 00.00.01

L3 4 SEA SSS FUL L1 ( 4 REACTIONS)

=> d 13, ibib abs crd, 1-4

L3 ANSWER 1 OF 4 CASREACT COPYRIGHT 2004 ACS on STN

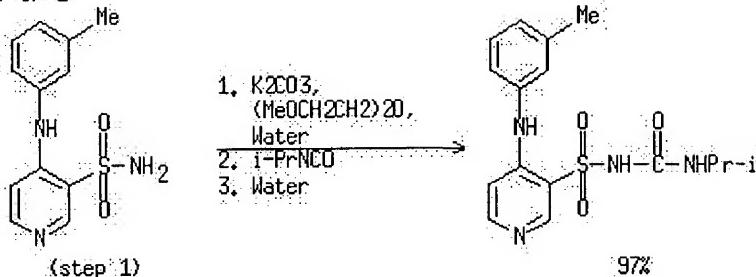
Full  Abstract  
 Text  References

ACCESSION NUMBER: 141:71454 CASREACT  
 TITLE: Process for the preparation of torsemide form II  
 INVENTOR(S): Lusanna, Massimiliano; Rainoni, Mauro; Gambuzza,  
 Filippo  
 PATENT ASSIGNEE(S): Cosma S.P.A., Italy  
 SOURCE: Eur. Pat. Appl., 28 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1433784	A1	20040630	EP 2003-29586	20031222
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2004138469	A1	20040715	US 2003-744613	20031222
<u>PRIORITY APPLN. INFO.:</u> <u>IT 2002-MI2749</u> 20021223				

AB The present invention relates to a new process for the prepn. of torsemide, in particular of pure and stable form II, which comprises direct synthesis of torsemide from 4-(3-methylphenylamino)-3-pyridine-sulfonamide. The new process envisages fewer steps than the processes described in the prior art, with improved yields and good quality from the chem. and preferably polymorphous points of view.

## RX(1) OF 1



NOTE: optimization study

REFERENCE COUNT:

5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 4 CASREACT COPYRIGHT 2004 ACS on STN

 Full   References  
 Text 

ACCESSION NUMBER:

139:197336 CASREACT

TITLE:

Synthesis of a new, curative and effective medicine for hypertension and diuretic torasemide

AUTHOR(S):

Xiong, Zhenhu; Fei, Xuening

CORPORATE SOURCE:

Tianjin Institute of Urban Construction, Tianjin, 300384, Peop. Rep. China

SOURCE:

Zhongguo Yaowu Huaxue Zazhi (2002), 12(4), 219-221, 224

CODEN: ZYHZEF; ISSN: 1005-0108

Zhongguo Yaowu Huaxue Zazhi Bianjibu

PUBLISHER:

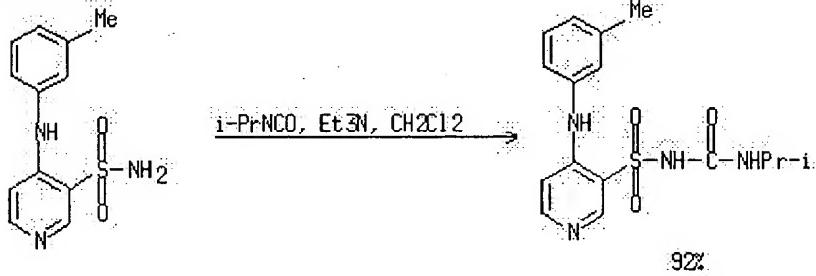
Journal

DOCUMENT TYPE:

Chinese

AB Torasemide was prep'd. in 5 steps with high yield from 4-hydroxypyridine by sulfonation, chlorination, amidation, substitution with 3-methylaniline, and condensation with iso-Pr isocyanate.

## RX(5) OF 15



L3 ANSWER 3 OF 4 CASREACT COPYRIGHT 2004 ACS on STN

 Full   References  
 Text 

ACCESSION NUMBER:

135:257163 CASREACT

TITLE:

Amidation process for preparing 4-chloro-3-pyridinesulfonamide and a method for the preparation of the diuretic torasemide

INVENTOR(S):

Kordova, Marco

PATENT ASSIGNEE(S):

Teva Pharmaceutical Industries Ltd., Israel; Teva Pharmaceuticals USA, Inc.

SOURCE:

PCT Int. Appl., 13 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

h

eb c

g cg b

cg

eb

LANGUAGE: English

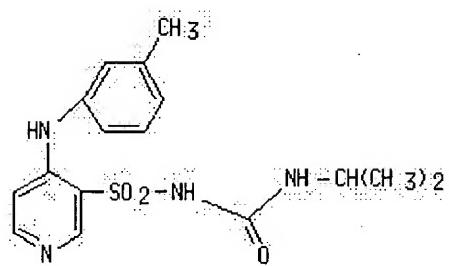
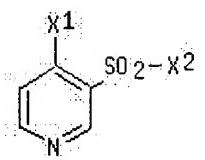
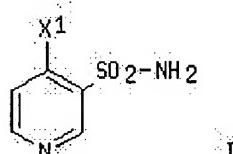
FAMILY ACC. NUM. COUNT: 1

## PATENT INFORMATION:

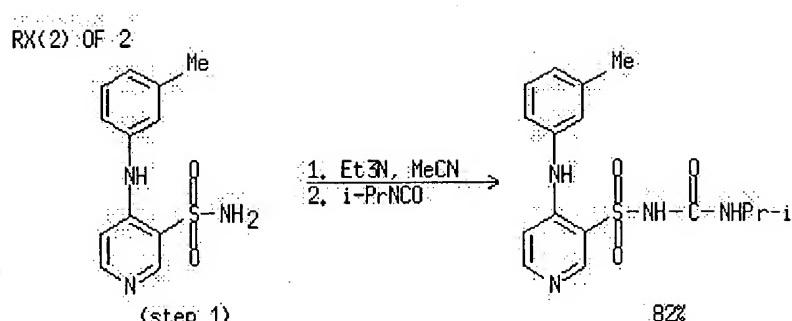
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001070226	A1	20010927	WO 2001-US8866	20010320
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002019537	A1	20020214	US 2001-812762	20010320
US 6635765	B2	20031021		
EP 1284733	A1	20030226	EP 2001-920556	20010320
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003527425	T2	20030916	JP 2001-568424	20010320
US 2003212277	A1	20031113	US 2003-428463	20030502
US 6670478	B2	20031230		
<u>PRIORITY APPLN. INFO.:</u>			<u>US 2000-190650P</u>	20000320
			<u>US 2000-211510P</u>	20000614
			<u>US 2001-812762</u>	20010320
			<u>WO 2001-US8866</u>	20010320

OTHER SOURCE(S): MARPAT 135:257163

GI



AB Torasemide intermediates (I; X1, X2 = Cl, F, Br) are prep'd. in high yield and selectivity by the amidation of a halopyridinesulfonyl halide (II) in an org. solvent with ammonia; torasemide (III) is prep'd. by the addn. reaction of I (X1 = 3-NHC6H4CH3) in the presence of NEt3 in acetonitrile with iso-Pr isocyanate.



**REFERENCE COUNT:**

4

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT.

1-3 ANSWER 4 OF 4 CASREACT COPYRIGHT 2004 ACS on STN

Full Text

ACCESSION NUMBER:

**PROCESS**

AUTHOR (S) :

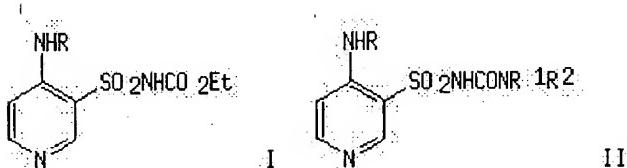
HONOR(S) :

CORPORATE SOURCE: Lab. Chim. Pharm., Inst. Pharm.  
SOURCE: European Journal of Medicinal C  
65-8  
CODEN: EJMC5; ISSN: 0009-4374

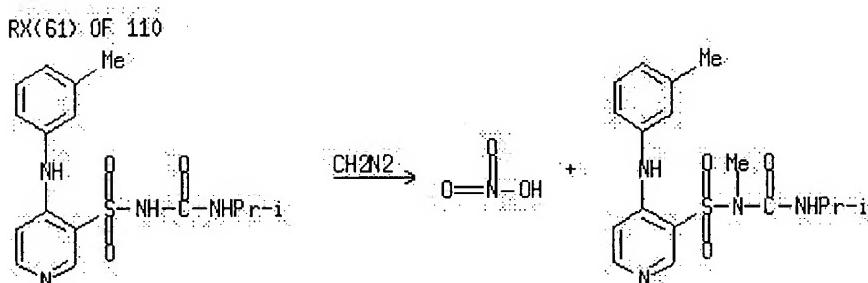
DOCUMENT TYPE: Journal

**DOCUMENT  
LANGUAGE:**

10



AB Carbamates I ( $R = \text{tolyl, ClC}_6\text{H}_4, \text{F}_3\text{CC}_6\text{H}_4, \text{Bu, cyclohexyl, PhCH}_2\text{CHMe}$ ), were treated with amines to yield (pyridinesulfonyl)ureas II [R same as above; R<sub>1</sub> = H, alkyl, allyl; R<sub>2</sub> = alkyl, allyl, piperidino, morpholino, N-(un)substituted piperidinyl, furfuryl, phenylalkyl, Ph, CH<sub>2</sub>CH<sub>2</sub>OH; or NR<sub>1</sub>R<sub>2</sub> = pyrrolidino, morpholino, piperidino, piperazino], which exhibited diuretic activity. I ( $R = m\text{-tolyl}$ ) was heated with CH<sub>2</sub>:CHCH<sub>2</sub>NH<sub>2</sub> and a mol. sieve in PhMe to give II ( $R = m\text{-tolyl}, R_1 = H, R_2 = \text{allyl}$ ).



=> file req

h                eb c            g cg    b            cg

eb

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	124.30	128.29
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.64	-2.64

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STRUCTURE FILE UPDATES: 31 AUG 2004 HIGHEST RN 736193-62-7  
 DICTIONARY FILE UPDATES: 31 AUG 2004 HIGHEST RN 736193-62-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>  
 L4 STRUCTURE uploaded

=> d 14  
 L4 HAS NO ANSWERS  
 L4 STR

=> s 14  
 SAMPLE SEARCH INITIATED 16:23:47 FILE 'REGISTRY'  
 SAMPLE SCREEN SEARCH COMPLETED - 14 TO ITERATE

100.0% PROCESSED 14 ITERATIONS 4 ANSWERS  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 56 TO 504  
 PROJECTED ANSWERS: 4 TO 200

L5 4 SEA SSS SAM L4

=> s 14 full  
 THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS  
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y  
 FULL SEARCH INITIATED 16:23:52 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 235 TO ITERATE

100.0% PROCESSED 235 ITERATIONS 66 ANSWERS  
 SEARCH TIME: 00.00.01

L6

66 SEA SSS FUL L4

```
=> file hcaplus
COST IN U.S. DOLLARS          SINCE FILE      TOTAL
                                ENTRY        SESSION
FULL ESTIMATED COST          156.26        284.55

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE      TOTAL
                                                ENTRY        SESSION
CA SUBSCRIBER PRICE           0.00         -2.64
```

FILE 'HCAPLUS' ENTERED AT 16:23:55 ON 01 SEP 2004  
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FILE COVERS 1907 - 1 Sep 2004 VOL 141 ISS 10  
 FILE LAST UPDATED: 31 Aug 2004 (20040831/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> s l5/prep
      3 L5
      3190662 PREP/RL
L7      2 L5/PREP
      (L5 (L) PREP/RL)
```

```
=> file reg
COST IN U.S. DOLLARS          SINCE FILE      TOTAL
                                ENTRY        SESSION
FULL ESTIMATED COST          2.36         286.91

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE      TOTAL
                                                ENTRY        SESSION
CA SUBSCRIBER PRICE           0.00         -2.64
```

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 DICTIONARY FILE UPDATES: 31 AUG 2004 HIGHEST RN 736193-62-7

h eb c g cg b cg

eb

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

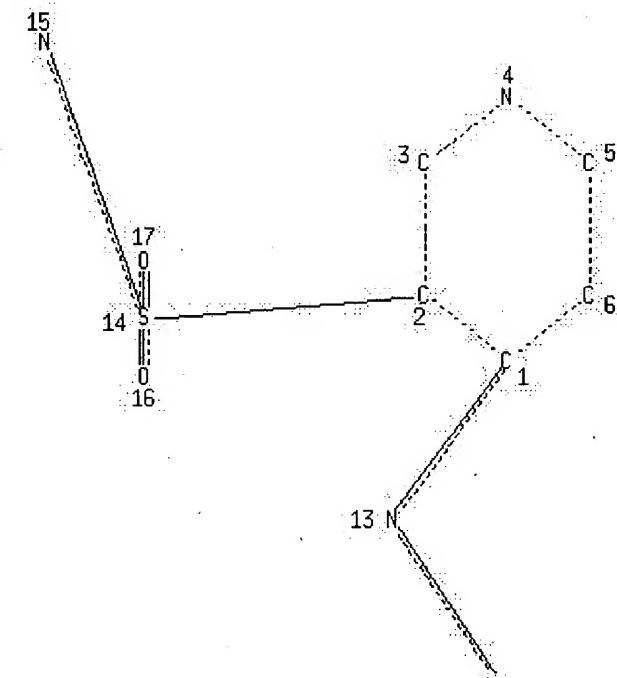
=>

L8 STRUCTURE UPLOADED

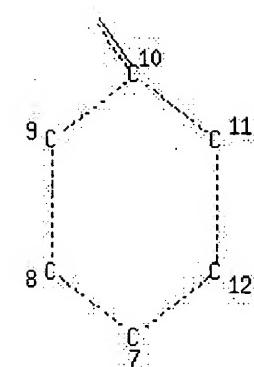
=> d 18

L8 HAS NO ANSWERS

L8 STR



Page 1-A



Page 2-A

NODE ATTRIBUTES:

NSPEC IS R AT 1  
NSPEC IS R AT 2

h eb c g cg b cg

eb

NSPEC IS R AT 3  
 NSPEC IS R AT 4  
 NSPEC IS R AT 5  
 NSPEC IS R AT 6  
 NSPEC IS R AT 7  
 NSPEC IS R AT 8  
 NSPEC IS R AT 9  
 NSPEC IS R AT 10  
 NSPEC IS R AT 11  
 NSPEC IS R AT 12  
 NSPEC IS C AT 13  
 NSPEC IS C AT 14  
 NSPEC IS C AT 15  
 NSPEC IS C AT 16  
 NSPEC IS C AT 17  
 DEFAULT MLEVEL IS ATOM  
 MLEVEL IS CLASS AT 13 14 15 16 17  
 DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

RSPEC I  
NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE

=> s 18  
SAMPLE SEARCH INITIATED 16:26:19 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 28 TO ITERATE

100.0% PROCESSED 28 ITERATIONS 12 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 243 TO 877  
PROJECTED ANSWERS: 33 TO 447

L9 12 SEA SSS SAM L8

=> s 18 full  
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y  
FULL SEARCH INITIATED 16:26:23 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 537 TO ITERATE

100.0% PROCESSED 537 ITERATIONS 259 ANSWERS  
SEARCH TIME: 00.00.01

L10 259 SEA SSS FUL L8

=> file hcaplus  
COST IN U.S. DOLLARS SINCE FILE TOTAL  
ENTRY SESSION  
FULL ESTIMATED COST 156.68 443.59  
  
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL  
ENTRY SESSION  
CA SUBSCRIBER PRICE 0.00 -2.64

FILE 'HCAPLUS' ENTERED AT 16:26:26 ON 01 SEP 2004  
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 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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FILE COVERS 1907 - 1 Sep 2004 VOL 141 ISS 10  
 FILE LAST UPDATED: 31 Aug 2004 (20040831/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> s l10/rct
      309 L10
      2653305 RCT/RL
L11      22 L10/RCT
          (L10 (L) RCT/RL)
```

=> d his

(FILE 'HOME' ENTERED AT 16:15:40 ON 01 SEP 2004)

FILE 'REGISTRY' ENTERED AT 16:15:45 ON 01 SEP 2004

FILE 'CASREACT' ENTERED AT 16:21:07 ON 01 SEP 2004

```
L1      STRUCTURE UPLOADED
L2      1 S L1
L3      4 S L1 FULL
```

FILE 'REGISTRY' ENTERED AT 16:22:23 ON 01 SEP 2004

```
L4      STRUCTURE UPLOADED
L5      4 S L4
L6      66 S L4 FULL
```

FILE 'HCAPLUS' ENTERED AT 16:23:55 ON 01 SEP 2004

```
L7      2 S L5/PREP
```

FILE 'REGISTRY' ENTERED AT 16:24:04 ON 01 SEP 2004

```
L8      STRUCTURE UPLOADED
L9      12 S L8
L10     259 S L8 FULL
```

FILE 'HCAPLUS' ENTERED AT 16:26:26 ON 01 SEP 2004

```
L11     22 S L10/RCT
```

=> s l11 and l7

```
L12     2 L11 AND L7
```

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.36	445.95
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.64

FILE 'REGISTRY' ENTERED AT 16:26:37 ON 01 SEP 2004  
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 31 AUG 2004 HIGHEST RN 736193-62-7  
 DICTIONARY FILE UPDATES: 31 AUG 2004 HIGHEST RN 736193-62-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>  
 L13 STRUCTURE uploaded

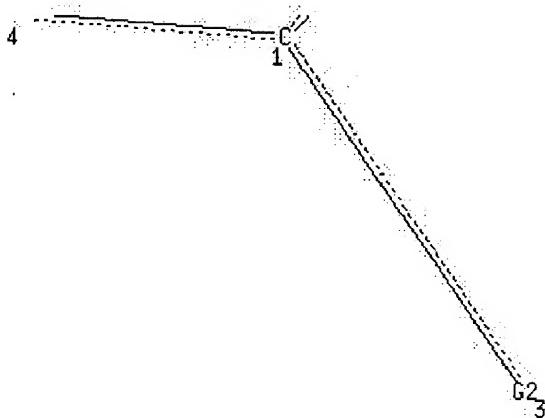
=> d 113  
 L13 HAS NO ANSWERS  
 L13 STR

10 11  
 9 C M3 C — C  
 M2 E3

07 58  
 Page 1-A

6 G1  
 5 C  
 N G2

Page 1-B



Page 2-B

VAR G1=7/8

VAR G2=9/10

## NODE ATTRIBUTES:

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HCOUNT IS M3      AT    9
HCOUNT IS M2      AT   10
HCOUNT IS E3      AT   11
NSPEC  IS C       AT    1
NSPEC  IS C       AT    2
NSPEC  IS C       AT    3
NSPEC  IS C       AT    4
NSPEC  IS C       AT    5
NSPEC  IS C       AT    6

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DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 1 4 5 7 8 9 10 11

DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE

=&gt; s l13

SAMPLE SEARCH INITIATED 16:28:24 FILE 'REGISTRY'  
 SAMPLE SCREEN SEARCH COMPLETED - 247027 TO ITERATE

0.4% PROCESSED 1000 ITERATIONS  
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
 SEARCH TIME: 00.00.01

20 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
 BATCH \*\*INCOMPLETE\*\*  
 PROJECTED ITERATIONS: EXCEEDS 1000000  
 PROJECTED ANSWERS: EXCEEDS 94596

L14 20 SEA SSS SAM L13

=> e isopropyl isocyanate/cn  
 E1 1 ISOPROPYL ISOBUTYL KETONE/CN  
 E2 1 ISOPROPYL ISOBUTYRATE/CN  
 E3 1 --> ISOPROPYL ISOCYANATE/CN  
 E4 1 ISOPROPYL ISOCYANIDE/CN

h eb c g cg b cg

eb

E5	1	ISOPROPYL ISOCYANIDE, COMPD. WITH TRIPHENYLBORANE/CN
E6	1	ISOPROPYL ISOCYANIDE, COMPD. WITH TRIPHENYLBORANE (1:1)/CN
E7	1	ISOPROPYL ISOCYANOACETATE/CN
E8	1	ISOPROPYL ISOHEXANOATE/CN
E9	1	ISOPROPYL ISOLAURATE/CN
E10	1	ISOPROPYL ISONITRILE/CN
E11	1	ISOPROPYL ISOPROPAETHIOLSULFINATE/CN
E12	1	ISOPROPYL ISOPROPOXYACETATE/CN

=> s e3  
L15 1 "ISOPROPYL ISOCYANATE"/CN

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	6.11	452.06
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.64

FILE 'HCAPLUS' ENTERED AT 16:28:55 ON 01 SEP 2004  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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FILE COVERS 1907 - 1 Sep 2004 VOL 141 ISS 10  
FILE LAST UPDATED: 31 Aug 2004 (20040831/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l15/rct  
961 L15  
2653305 RCT/RL  
L16 838 L15/RCT  
(L15 (L) RCT/RL)

=> d his

(FILE 'HOME' ENTERED AT 16:15:40 ON 01 SEP 2004)

FILE 'REGISTRY' ENTERED AT 16:15:45 ON 01 SEP 2004

FILE 'CASREACT' ENTERED AT 16:21:07 ON 01 SEP 2004

L1	STRUCTURE UPLOADED
L2	1 S L1
L3	4 S L1 FULL

FILE 'REGISTRY' ENTERED AT 16:22:23 ON 01 SEP 2004  
L4 STRUCTURE uploaded  
L5 4 S L4  
L6 66 S L4 FULL

FILE 'HCAPLUS' ENTERED AT 16:23:55 ON 01 SEP 2004  
L7 2 S L5/PREP

FILE 'REGISTRY' ENTERED AT 16:24:04 ON 01 SEP 2004  
L8 STRUCTURE uploaded  
L9 12 S L8  
L10 259 S L8 FULL

FILE 'HCAPLUS' ENTERED AT 16:26:26 ON 01 SEP 2004  
L11 22 S L10/RCT  
L12 2 S L11 AND L7

FILE 'REGISTRY' ENTERED AT 16:26:37 ON 01 SEP 2004  
L13 STRUCTURE uploaded  
L14 20 S L13  
E ISOPROPYL ISOCYANATE/CN  
L15 1 S E3

FILE 'HCAPLUS' ENTERED AT 16:28:55 ON 01 SEP 2004  
L16 838 S L15/RCT

=> s l16 and l12  
L17 1 L16 AND L12

=> d l17, ihib abs hitstr, 1

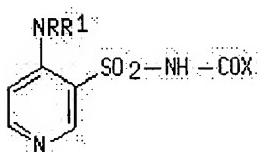
L17 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full  Structure  
 Text  References

ACCESSION NUMBER: 1980:128730 HCAPLUS  
DOCUMENT NUMBER: 92:128730  
TITLE: 4-Amino-3-sulfamoylpyridine derivatives and their use  
INVENTOR(S): Lapierre, Charles; Delarge, Jacques; Thunus, Leopold;  
Georges, Andre; De Ridder, Rene; Ghys, Arlette  
PATENT ASSIGNEE(S): Christiaens, A., S. A., Belg.  
SOURCE: Eur. Pat. Appl., 32 pp.  
CODEN: EPXXDW  
DOCUMENT TYPE: Patent  
LANGUAGE: French  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
<u>EP 3383</u>	A2	19790808	<u>EP 1979-200037</u>	19790122
<u>EP 3383</u>	A3	19790905		
<u>EP 3383</u>	B1	19830209		
R: DE, NL, SE				
<u>GB 1593609</u>	A	19810722	<u>GB 1978-3918</u>	19780131
<u>ES 476658</u>	A1	19790716	<u>ES 1979-476658</u>	19790109
<u>ZA 7900090</u>	A	19801029	<u>ZA 1979-90</u>	19790109
<u>IL 56407</u>	A1	19830515	<u>IL 1979-56407</u>	19790110
<u>AU 7943317</u>	A1	19790809	<u>AU 1979-43317</u>	19790112
<u>AU 524287</u>	B2	19820909		

CA 1124720	A1	19820601	CA 1979-319934	19790119
BE 873656	A1	19790723	BE 1979-193040	19790123
US 4244950	A	19810113	US 1979-6154	19790124
FR 2416225	A1	19790831	FR 1979-2109	19790126
FR 2416225	B1	19811106		
AT 7900594	A	19840115	AT 1979-594	19790126
AT 375646	B	19840827		
DD 141309	C	19800423	DD 1979-210692	19790129
HU 20570	O	19810828	HU 1979-CI1905	19790130
HU 178203	P	19820328		
<u>PRIORITY APPLN. INFO.:</u>				
CASREACT 92:128730				
OTHER SOURCE(S):				
GI				



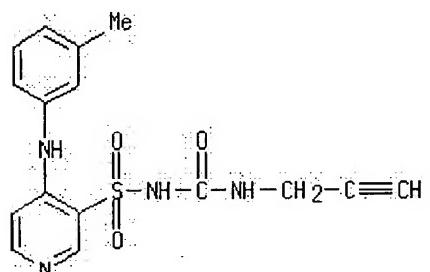
AB Diuretic sulfamoylpyridines I [R = H, alkyl, cycloalkyl, R<sub>2</sub>R<sub>3</sub>NCO, R<sub>2</sub>R<sub>3</sub>NSO<sub>2</sub> (R<sub>2</sub>, R<sub>3</sub> = alkyl; R<sub>2</sub>R<sub>3</sub>N = heterocyclyl); R<sub>1</sub> = alkyl, haloalkyl, cycloalkyl, alkenyl, Ph, phenylalkyl, Ph<sub>2</sub>CH<sub>2</sub>, isobornyl, furfuryl, dialkylaminoalkyl; X = substituted amino, alkoxy or heterocyclyl] were prepd. and showed diuretic activity at 25 mg/kg. in mice. Thus, refluxing 3-sulfamido-4-chloropyridine with 3-MeC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>NH<sub>2</sub> in EtOH 9 h gave 3-sulfamido-4-(3-methylbenzyl)aminopyridine, which was treated with Me<sub>2</sub>CHNCO in CH<sub>2</sub>Cl<sub>2</sub> contg. Et<sub>3</sub>N 20 h at room temp. to give I (R = H, R<sub>1</sub> = 3-MeC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>, X = Me<sub>2</sub>CHNH).

IT 72811-00-8P 72811-63-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. and diuretic activity of)

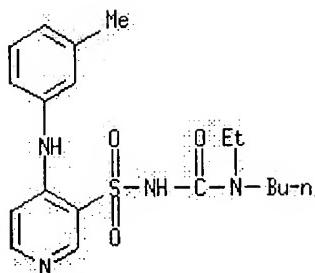
RN 72811-00-8 HCPLUS

CN 3-Pyridinesulfonamide, 4-[(3-methylphenyl)amino]-N-[(2-propynylamino)carbonyl]- (9CI) (CA INDEX NAME)



RN 72811-63-3 HCPLUS

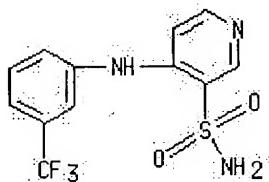
CN 3-Pyridinesulfonamide, N-[(butylethylamino)carbonyl]-4-[(3-methylphenyl)amino]- (9CI) (CA INDEX NAME)

IT 38030-43-2P 72810-58-3P

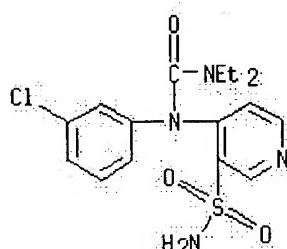
RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation); RACT (Reactant or reagent)  
 (prepn. and reaction of, with Et isocyanate)

RN 38030-43-2 HCPLUS

CN 3-Pyridinesulfonamide, 4-[[3-(trifluoromethyl)phenyl]amino]- (9CI) (CA INDEX NAME)

RN 72810-58-3 HCPLUS

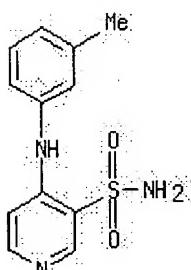
CN 3-Pyridinesulfonamide, 4-[(3-chlorophenyl)[(diethylamino)carbonyl]amino]-  
 (9CI) (CA INDEX NAME)

IT 72811-73-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation); RACT (Reactant or reagent)  
 (prepn. and reaction of, with isopropylisocyanate)

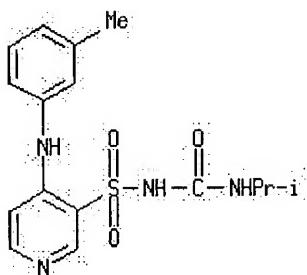
RN 72811-73-5 HCPLUS

CN 3-Pyridinesulfonamide, 4-[(3-methylphenyl)amino]- (9CI) (CA INDEX NAME)

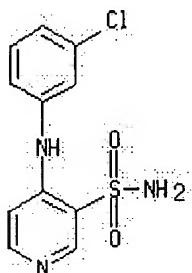
IT 72810-59-4

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with di-Et carbamoyl chloride)

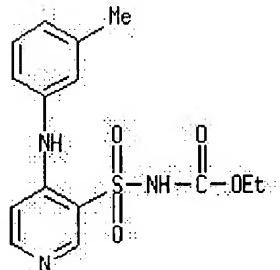
RN 72810-59-4 HCAPLUS  
 CN 3-Pyridinesulfonamide, N-[(1-methylethyl)amino]carbonyl]-4-[(3-methylphenyl)amino]-, sodium salt (9CI) (CA INDEX NAME)



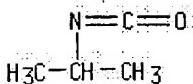
# x Na  
 IT 52214-13-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with diethylcarbamoyl chloride)  
 RN 52214-13-8 HCAPLUS  
 CN 3-Pyridinesulfonamide, 4-[(3-chlorophenyl)amino]- (9CI) (CA INDEX NAME)



IT 72810-57-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with methylbutylamine)  
 RN 72810-57-2 HCAPLUS  
 CN Carbamic acid, [(4-[(3-methylphenyl)amino]-3-pyridinyl)sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)



IT 1795-48-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with sulfamoyl(methylbenzyl)aminopyridine)  
 RN 1795-48-8 HCAPLUS  
 CN Propane, 2-isocyanato- (9CI) (CA INDEX NAME)



RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with sulfamoylaminopyridines)

=> d his

(FILE 'HOME' ENTERED AT 16:15:40 ON 01 SEP 2004)

FILE 'REGISTRY' ENTERED AT 16:15:45 ON 01 SEP 2004

FILE 'CASREACT' ENTERED AT 16:21:07 ON 01 SEP 2004

L1                   STRUCTURE UPLOADED  
L2                   1 S L1  
L3                   4 S L1 FULL

FILE 'REGISTRY' ENTERED AT 16:22:23 ON 01 SEP 2004

L4                   STRUCTURE UPLOADED  
L5                   4 S L4  
L6                   66 S L4 FULL

FILE 'HCAPLUS' ENTERED AT 16:23:55 ON 01 SEP 2004

L7                   2 S L5/PREP

FILE 'REGISTRY' ENTERED AT 16:24:04 ON 01 SEP 2004

L8                   STRUCTURE UPLOADED  
L9                   12 S L8  
L10                  259 S L8 FULL

FILE 'HCAPLUS' ENTERED AT 16:26:26 ON 01 SEP 2004

L11                  22 S L10/RCT  
L12                  2 S L11 AND L7

FILE 'REGISTRY' ENTERED AT 16:26:37 ON 01 SEP 2004

L13                  STRUCTURE UPLOADED  
L14                  20 S, L13  
                      E ISOPROPYL ISOCYANATE/CN  
L15                  1 S E3

FILE 'HCAPLUS' ENTERED AT 16:28:55 ON 01 SEP 2004

L16                  838 S L15/RCT  
L17                  1 S L16 AND L12

=> s l12 not l17

L18                  1 L12 NOT L17

=> d l18, ibib abs hitstr, 1

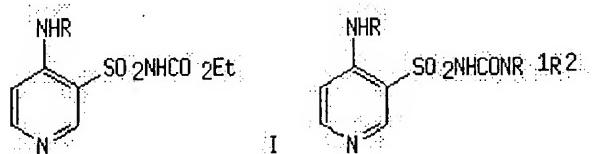
L18 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full  Search  
 Text  References

ACCESSION NUMBER:       1981:174826 HCAPLUS  
 DOCUMENT NUMBER:       94:174826  
 TITLE:                  New diuretic torasemide derivatives  
 AUTHOR(S):             Delarge, Jacques; Lapierre, C. L.; De Ridder, Rene;  
                          Ghys, Arlette  
 CORPORATE SOURCE:      Lab. Chim. Pharm., Inst. Pharm., Liege, B-4000, Belg.

SOURCE: European Journal of Medicinal Chemistry (1981), 16(1),  
65-8  
CODEN: EJMCA5; ISSN: 0009-4374

DOCUMENT TYPE: Journal  
LANGUAGE: French  
OTHER SOURCE(S): CASREACT 94:174826  
GI



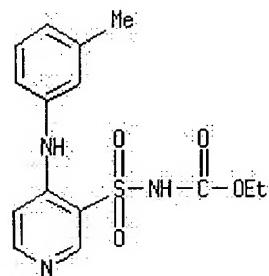
AB Carbamates I (R = tolyl, ClC<sub>6</sub>H<sub>4</sub>, F<sub>3</sub>C<sub>6</sub>H<sub>4</sub>, Bu, cyclohexyl, PhCH<sub>2</sub>CHMe), were treated with amines to yield (pyridinesulfonyl)ureas II [R same as above; R<sub>1</sub> = H, alkyl, allyl; R<sub>2</sub> = alkyl, allyl, piperidino, morpholino, N-(un)substituted piperidinyl, furfuryl, phenylalkyl, Ph, CH<sub>2</sub>CH<sub>2</sub>OH; or NR<sub>1</sub>R<sub>2</sub> = pyrrolidino, morpholino, piperidino, piperazinol], which exhibited diuretic activity. I (R = m-tolyl) was heated with CH<sub>2</sub>:CHCH<sub>2</sub>NH<sub>2</sub> and a mol. sieve in PhMe to give II (R = m-tolyl, R<sub>1</sub> = H, R<sub>2</sub> = allyl).

IT 72810-57-2 72811-25-7 72811-26-8

RL: RCT (Reactant); RACT (Reactant or reagent)  
(amidation of)

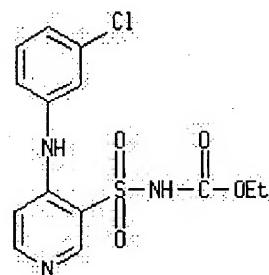
RN 72810-57-2 HCPLUS

CN Carbamic acid, [[4-[(3-methylphenyl)amino]-3-pyridinyl]sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)



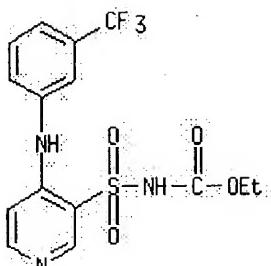
RN 72811-25-7 HCPLUS

CN Carbamic acid, [[4-[(3-chlorophenyl)amino]-3-pyridinyl]sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 72811-26-8 HCPLUS

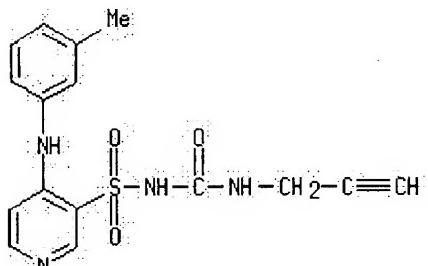
CN Carbamic acid, [[4-[[3-(trifluoromethyl)phenyl]amino]-3-pyridinyl]sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)

IT 72811-00-8P 72811-63-3P 77281-87-9P

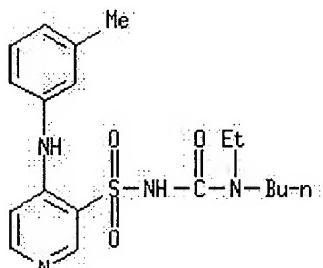
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)  
(prepn. and diuretic activity of)

RN 72811-00-8 HCPLUS

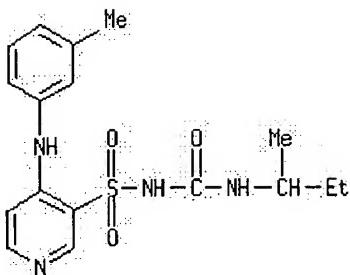
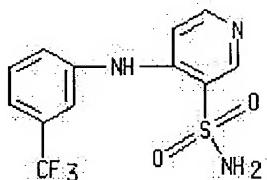
CN 3-Pyridinesulfonamide, 4-[(3-methylphenyl)amino]-N-[(2-propynylamino)carbonyl]- (9CI) (CA INDEX NAME)

RN 72811-63-3 HCPLUS

CN 3-Pyridinesulfonamide, N-[(butylethylamino)carbonyl]-4-[(3-methylphenyl)amino]- (9CI) (CA INDEX NAME)

RN 77281-87-9 HCPLUS

CN 3-Pyridinesulfonamide, 4-[(3-methylphenyl)amino]-N-[[[(1-methylpropyl)amino]carbonyl]- (9CI) (CA INDEX NAME)

IT 38030-43-2RL: RCT (Reactant); RACT (Reactant or reagent)  
(N-mesylation of)RN 38030-43-2 HCAPLUSCN 3-Pyridinesulfonamide, 4-[[3-(trifluoromethyl)phenyl]amino]- (9CI) (CA  
INDEX NAME)

=&gt; file caold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	11.88	463.94
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.40	-4.04

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the 'REGISTRY' file. Enter HELP FIRST for more information.

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(FILE 'HOME' ENTERED AT 16:15:40 ON 01 SEP 2004)

FILE 'REGISTRY' ENTERED AT 16:15:45 ON 01 SEP 2004

FILE 'CASREACT' ENTERED AT 16:21:07 ON 01 SEP 2004  
L1                   STRUCTURE uploaded  
L2                   1 S L1  
L3                   4 S L1 FULL

FILE 'REGISTRY' ENTERED AT 16:22:23 ON 01 SEP 2004  
L4                   STRUCTURE uploaded  
L5                   4 S L4  
L6                   66 S L4 FULL

FILE 'HCAPLUS' ENTERED AT 16:23:55 ON 01 SEP 2004  
L7                   2 S L5/PREP

FILE 'REGISTRY' ENTERED AT 16:24:04 ON 01 SEP 2004  
L8                   STRUCTURE uploaded  
L9                   12 S L8  
L10                  259 S L8 FULL

FILE 'HCAPLUS' ENTERED AT 16:26:26 ON 01 SEP 2004  
L11                  22 S L10/RCT  
L12                  2 S L11 AND L7

FILE 'REGISTRY' ENTERED AT 16:26:37 ON 01 SEP 2004  
L13                  STRUCTURE uploaded  
L14                  20 S L13  
                      E ISOPROPYL ISOCYANATE/CN  
L15                  1 S E3

FILE 'HCAPLUS' ENTERED AT 16:28:55 ON 01 SEP 2004  
L16                  838 S L15/RCT  
L17                  1 S L16 AND L12  
L18                  1 S L12 NOT L17

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=> s l6 and l10  
      0 L6  
      0 L10  
L19                  0 L6 AND L10

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<u>NEWS</u>	<u>1</u>	Web Page URLs for STN Seminar Schedule - N. America "Ask CAS" for self-help around the clock
<u>NEWS</u>	<u>2</u>	
<u>NEWS</u>	<u>3</u>	May 12 EXTEND option available in structure searching
<u>NEWS</u>	<u>4</u>	May 12 Polymer links for the POLYLINK command completed in REGISTRY
<u>NEWS</u>	<u>5</u>	May 27 New UPM (Update Code Maximum) field for more efficient patent SDIs in CAplus
<u>NEWS</u>	<u>6</u>	May 27 CAplus super roles and document types searchable in REGISTRY
<u>NEWS</u>	<u>7</u>	Jun 28 Additional enzyme-catalyzed reactions added to CASREACT
<u>NEWS</u>	<u>8</u>	Jun 28 ANTE, AQUALINE, BIOENG, CIVILENG, ENVIROENG, MECHENG, and WATER from CSA now available on STN(R)
<u>NEWS</u>	<u>9</u>	Jul 12 BEILSTEIN enhanced with new display and select options, resulting in a closer connection to BABS
<u>NEWS</u>	<u>10</u>	Jul 30 BEILSTEIN on STN workshop to be held August 24 in conjunction with the 228th ACS National Meeting
<u>NEWS</u>	<u>11</u>	AUG 02 IFIPAT/IFIUDB/IFICDB reloaded with new search and display fields
<u>NEWS</u>	<u>12</u>	AUG 02 CAplus and CA patent records enhanced with European and Japan Patent Office Classifications
<u>NEWS</u>	<u>13</u>	AUG 02 STN User Update to be held August 22 in conjunction with the 228th ACS National Meeting
<u>NEWS</u>	<u>14</u>	AUG 02 The Analysis Edition of STN Express with Discover! (Version 7.01 for Windows) now available
<u>NEWS</u>	<u>15</u>	AUG 04 Pricing for the Save Answers for SciFinder Wizard within STN Express with Discover! will change September 1, 2004
<u>NEWS</u>	<u>16</u>	AUG 27 BIOCOMMERCE: Changes and enhancements to content coverage
<u>NEWS</u>	<u>17</u>	AUG 27 BIOTECHABS/BIOTECHDS: Two new display fields added for legal status data from INPADOC
<u>NEWS</u>	<u>18</u>	SEP 01 INPADOC: New family current-awareness alert (SDI) available
<u>NEWS</u>	<u>19</u>	SEP 01 New pricing for the Save Answers for SciFinder Wizard within STN Express with Discover!
<u>NEWS</u>	<u>20</u>	SEP 01 New display format, HITSTR, available in WPIDS/WPINDEX/WPIX

<u>NEWS EXPRESS</u>	JULY 30 CURRENT WINDOWS VERSION IS V7.01, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
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FILE COVERS 1907 - 1 Sep 2004 VOL 141 ISS 10  
THIS PAGE UPDATED 21 Jun 2004 (20040831/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s torsemide

=> s l1 and polymorph?  
155749 POLYMORPH?  
L2 8 L1 AND POLYMORPH?

=> s 12 and review/dt  
1754103 REVIEW/DT  
L3 2 L2 AND REVIEW/DT

$\Rightarrow$  Q 13, ibib abs., 1-2

L3 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text

ACCESSION NUMBER: 2000:352882 HCAPLUS  
DOCUMENT NUMBER: 133:83770  
TITLE: **Torsemide** metabolism by CYP2C9 variants and other

AUTHOR(S): Miners, John O.; Coulter, Sally; Birkett, Donald J.; Goldstein, Joyce A.

CORPORATE SOURCE: Department of Clinical Pharmacology, Flinders Medical Centre and Flinders, University School of Medicine, Adelaide, Australia

SOURCE: Pharmacogenetics (2000), 10(3)  
CODEN: PHMCEE; ISSN: 0960-314

PUBLISHER: Lippincott Williams & Wilkins

DOCUMENT TYPE: Journal

LANGUAGE: English  
AB A review with 19 refs. This review describes studies which investigated **torsemide** methylhydroxylation by the CYP2C9 variants to det. possible effects of CYP2C9 **polymorphism** on **torsemide** elimination in vivo, as well as studies with recombinant CYP 2C8, 2C18 and 2C19 to confirm the isoform selectivity of **torsemide** methylhydroxylation and sulphaphenazole inhibition.

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

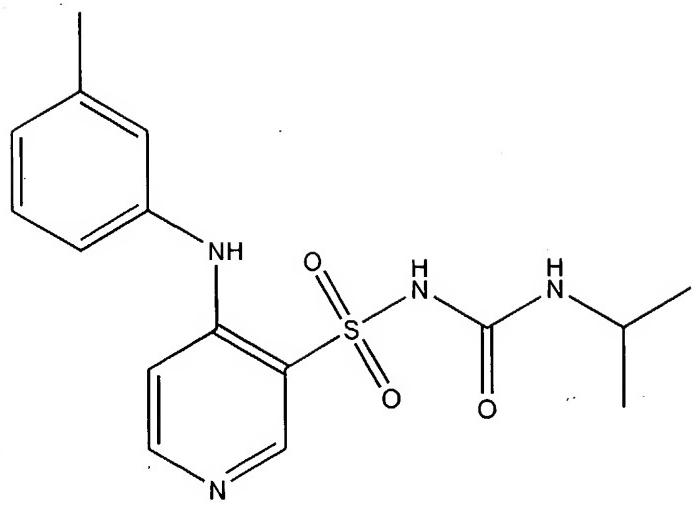
Full  Abstract  
 Text  References

ACCESSION NUMBER: 1998:412144 HCAPLUS  
 DOCUMENT NUMBER: 129:183680  
 TITLE: Cytochrome P 450 2C9: an enzyme of major importance in human drug metabolism  
 AUTHOR(S): Miners, John O.; Birkett, Donald J.  
 CORPORATE SOURCE: Department of Clinical Pharmacology, Flinders Medical Centre and Flinders University School of Medicine, Bedford Park, SA 5042, Australia  
 SOURCE: British Journal of Clinical Pharmacology (1998), 45(6), 525-538  
 CODEN: BCPHBM; ISSN: 0306-5251  
 PUBLISHER: Blackwell Science Ltd.  
 DOCUMENT TYPE: Journal; General Review  
 LANGUAGE: English

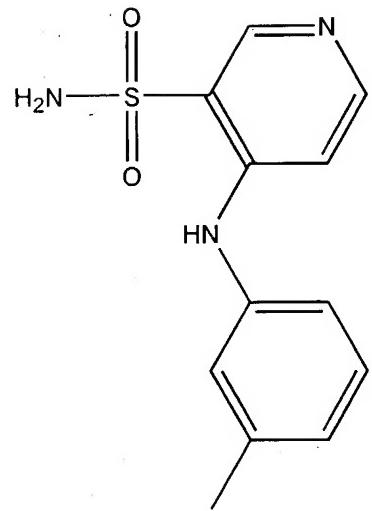
AB A review with 154 refs. Accumulating evidence indicates that cytochrome P 450 2C9 (CYP2C9) ranks among the most important drug-metabolizing enzymes in humans. Substrates for CYP2C9 include fluoxetine, losartan, phenytoin, tolbutamide, **torsemide**, S-warfarin, and numerous NSAIDs. CYP2C9 activity in vivo is inducible by rifampicin. Evidence suggests that CYP2C9 substrates may also be induced variably by carbamazepine, ETOH, and phenobarbitone. Apart from the mutual competitive inhibition which may occur between alternate substrates, numerous other drugs have been shown to inhibit CYP2C9 activity in vivo and/or in vitro. Clin. significant inhibition may occur with co-administration of amiodarone, fluconazole, phenylbutazone, sulphapyrazone, sulphaphenazole, and certain other sulfonamides. **Polymorphisms** in the coding region of the CYP2C9 gene produce variants at amino acid residues 144 (R144C) and 359 (I359L) of the CYP2C9 protein. Individuals homozygous for Leu-359 have markedly diminished metabolic capacities for most CYP2C9 substrates, although the frequency of this allele is relatively low. Consistent with the modulation of enzyme activity by genetic and other factors, wide interindividual variability occurs in the elimination and/or dosage requirements of prototypic CYP2C9 substrates. Individualization of dose is essential for those CYP2C9 substrates with a narrow therapeutic index.

REFERENCE COUNT: 154 THERE ARE 154 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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N-[(1-methylethyl)amino]carbonyl]-4-[(3-methylphenyl)amino]-3-pyridinesulfonamide



4-[(3-methylphenyl)amino]-3-pyridinesulfonamide

